

METHODS AND APPARATUS FOR MASS FINGERPRINTING OF BIOMOLECULES

ABSTRACT

5 Methods and apparatus that determine molecules in a sample by mass
fingerprinting are disclosed. In one embodiment, the method comprises: (1) comparing
the mass signals of a mass spectrum to a biomolecule fragment signal list to determine
mass signal-biomolecule fragment matches; (2) quantifying the mass signal-biomolecule
fragment match significance based on a biomolecule fragment detection parameter; (3)
10 quantifying a biomolecule's likelihood of being present in the sample based on the
quantified significance of mass signal-biomolecule fragment matches; and (4)
determining the likelihood of the presence of biomolecule(s) in the sample by comparison
of the quantified biomolecule presence likelihood. The invention also provides an
apparatus for determining the likelihood of the presence of a biomolecule in a sample
15 using the biomolecule fragment detection parameters of biomolecule fragments matched
to the mass signals of a mass spectrum of the sample.

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